### Hybrid Van Der Waals Materials In Next-Generation Electronics



Completed Technology Project (2015 - 2019)

#### **Project Introduction**

In nature, there exists a class of materials which are inherently twodimensional (2D). Although they form solid 3D structures, the individual atoms have strong bonds in one plane, and weak bonds out of plane; a single sheet can be separated from the bulk. These are called van der Waals (VDW) materials. 2D and VDW materials will be extremely useful to NASA in many electronic and optical devices due to their low weight and high efficiency. Throughout this proposal, I will discuss the unique properties of 2D and VDW materials, and the opportunities to combine multiple 2D materials into a hybrid metamaterial. A multi-functional solid state device can be constructed by the stacking of different-function 2D layers. The 2D layers can participate in conduction, insulation, light-matter interactions, ion storage, catalysis, charge storage, and coupling. The questions that need to be answered are: (i) how does hybridization alter the properties of the layer; (ii) can we form hybrids with layers which behave independently; (iii) and do unique properties exist in hybrids which do not manifest in homogeneous VDW materials? To answer these questions requires probing hybrids with differing composition and geometry. Synthesis of a wide range of hybrid VDW materials is not possible without being overly expensive and time consuming. But, manufacturing a specific material cheaply and efficiently is certainly possible. Additionally, the computational and theoretical techniques we will use are widely applicable; we can calculate a hybrid's electronic and optical properties and easily switch to study a hybrid with significantly different elemental makeup and hybridization. I will perform analytical calculations, modeling, and Density Functional Theory (DFT) studies to answer the above questions, and I will use our results to motivate the synthesis of new materials for devices that are of interest to NASA.

#### **Anticipated Benefits**

This project investigates the unique properties of 2D and VDW materials, and the opportunities to combine multiple 2D materials into a hybrid metamaterial. A multi-functional solid state device can be constructed by the stacking of different-function 2D layers. The 2D layers can participate in conduction, insulation, light-matter interactions, ion storage, catalysis, charge storage, and coupling. This project includes analytical calculations, modeling, and Density Functional Theory (DFT) studies, and project results could be used to motivate the synthesis of new materials for devices that are of interest to NASA.



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#### **Primary U.S. Work Locations and Key Partners**



Organizations Performing Work	Role	Туре	Location
University of Notre Dame(Notre Dame)	Lead Organization	Academia	Notre Dame, Indiana
Jet Propulsion Laboratory(JPL)	Supporting Organization	NASA Center	Pasadena, California

### **Primary U.S. Work Locations**

Indiana

#### **Project Website:**

https://www.nasa.gov/strg#.VQb6T0jJzyE

## Organizational Responsibility

# Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

#### **Lead Organization:**

University of Notre Dame (Notre Dame)

#### **Responsible Program:**

Space Technology Research Grants

### **Project Management**

#### **Program Director:**

Claudia M Meyer

#### **Program Manager:**

Hung D Nguyen

#### **Principal Investigator:**

Boldizsar Janko

#### **Co-Investigator:**

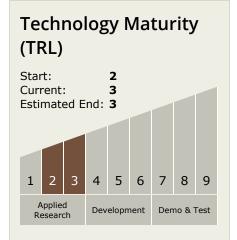
Anthony J Ruth



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### **Technology Areas**

#### **Primary:**

- TX12 Materials, Structures, Mechanical Systems, and Manufacturing
  - └ TX12.1 Materials
    - ☐ TX12.1.6 Materials for Electrical Power Generation, Energy Storage, Power Distribution and Electrical Machines

### **Target Destination**

Outside the Solar System

